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Toward a switchable molecular rotor. Unexpected dynamic behavior of functionalized overcrowded alkenes

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Table 1. Results of coalescence spectroscopy of alkene **1** in DMSO-d₆

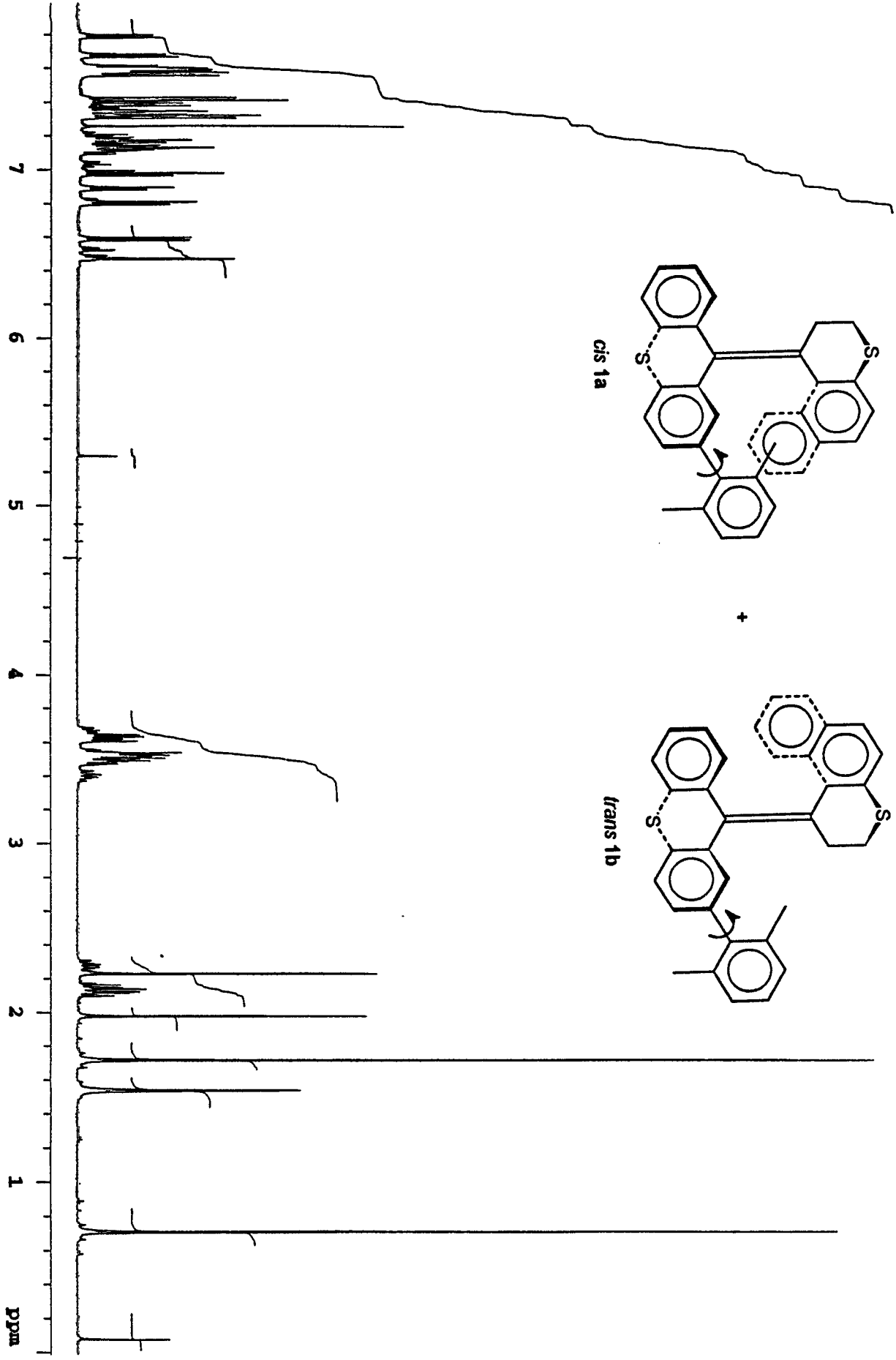
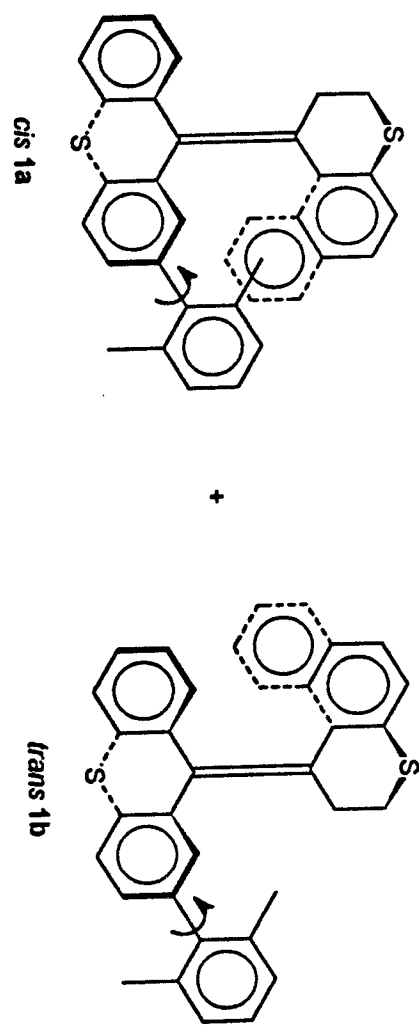
T(K)	<i>cis</i> 1a $\Delta\nu$ (Hz)	<i>trans</i> 1b $\Delta\nu$ (Hz)
313	291.0	79.4
323	288.8	79.4
333	286.5	79.9
343	284.3	80.3
353	281.2	80.3
363	278.9	80.5
373	275.3	80.5
383	274.9	81.0
393	270	82
403	270	82
413	264	82
423	255	80
433	231	80
443	204	78

Table 2. Results of Exchange Spectroscopy of *cis* **1a** in DMSO-d₆.

<i>T</i> (K)	<i>k</i> (s ⁻¹)	Δ <i>G</i> [*] (kcal.mol ⁻¹)
303	0.119	19.0 ± 0.2
313	0.264	19.2 ± 0.2
323	0.580	19.3 ± 0.2
343	2.310	19.6 ± 0.2
363	7.795	19.9 ± 0.2

Table 3. Results of Exchange Spectroscopy on *trans* **1b** in DMSO-d₆.

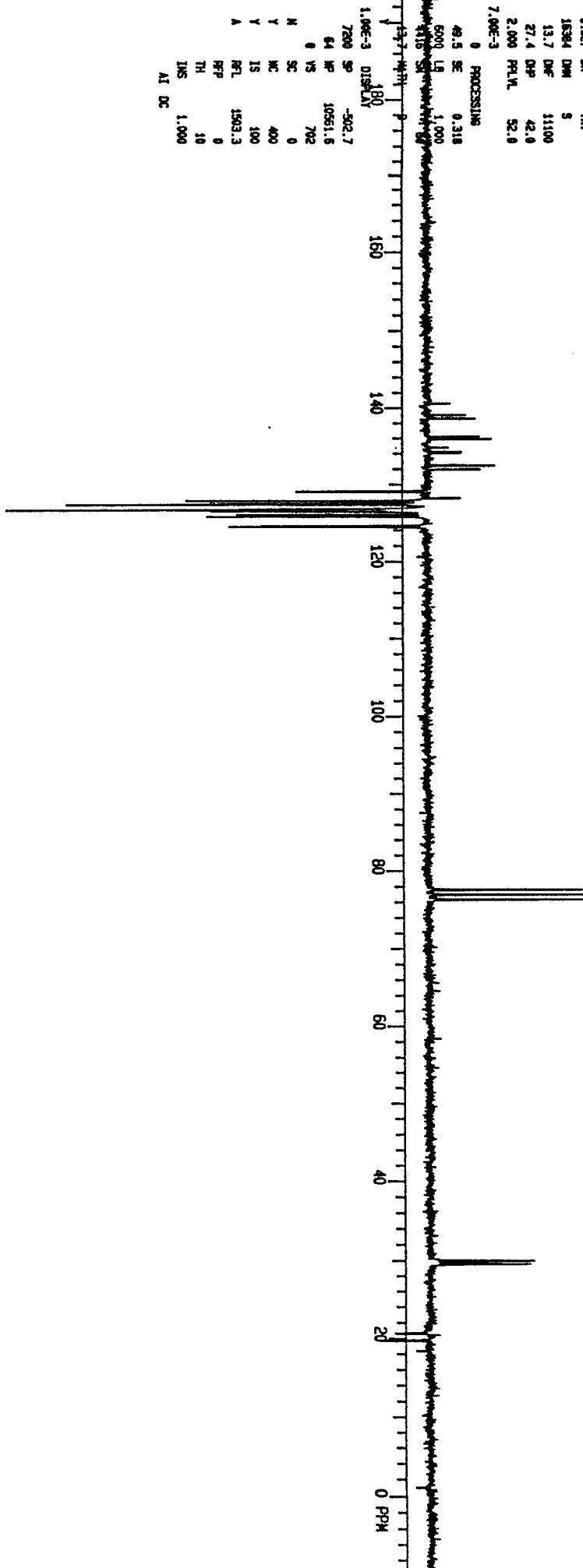
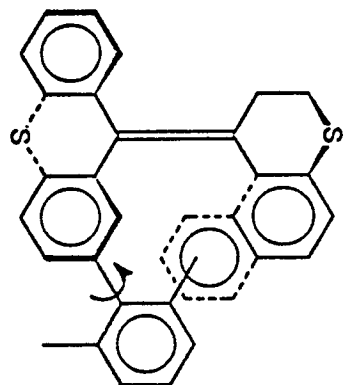
<i>T</i> (K)	<i>k</i> (s ⁻¹)	Δ <i>G</i> [*] (kcal.mol ⁻¹)
303	0.038	19.7 ± 0.2
313	0.100	19.8 ± 0.2
323	0.221	19.9 ± 0.2
343	1.105	20.1 ± 0.2
363	3.953	20.4 ± 0.2

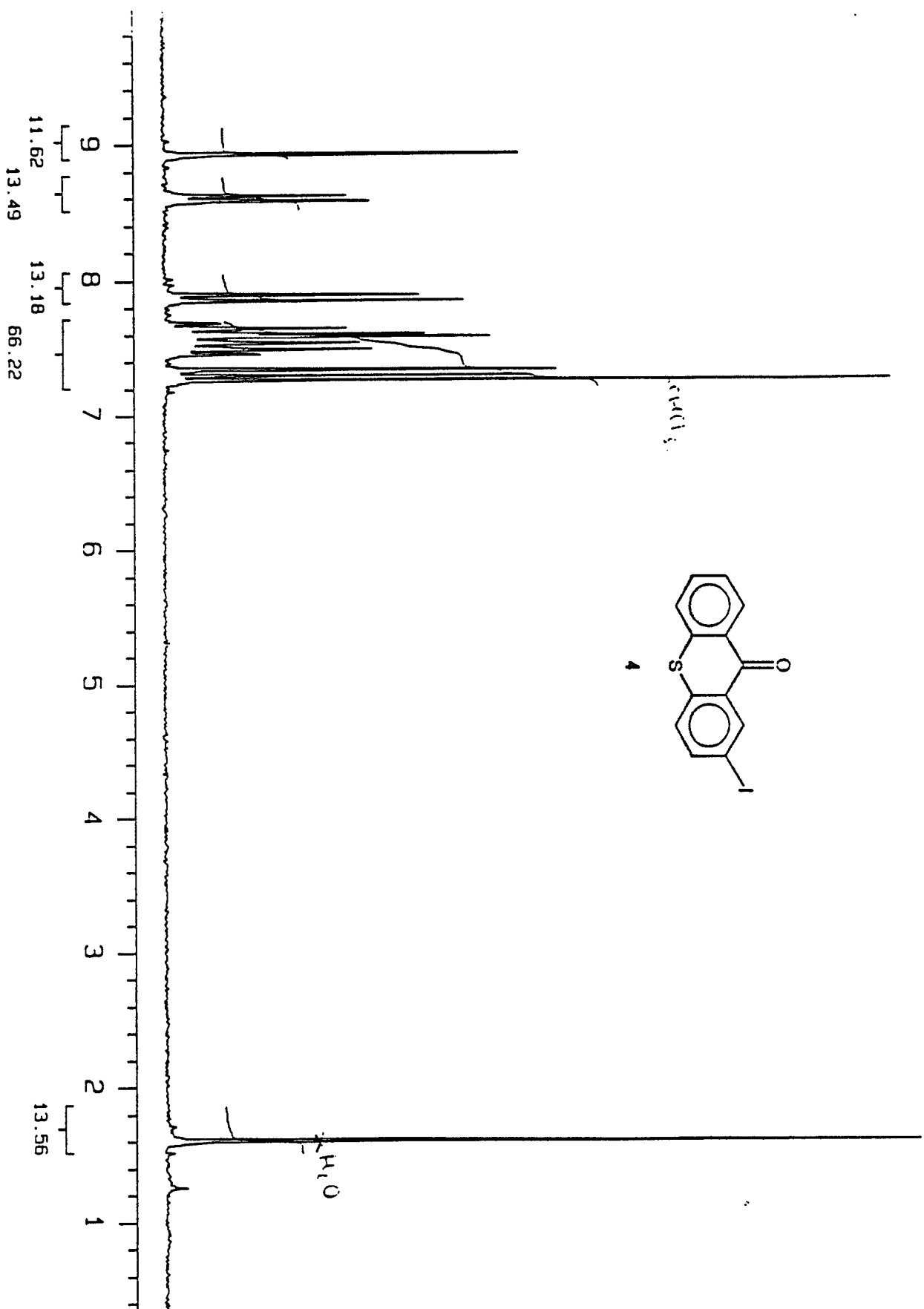
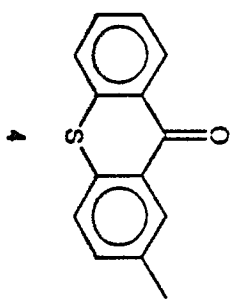


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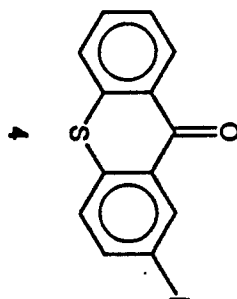
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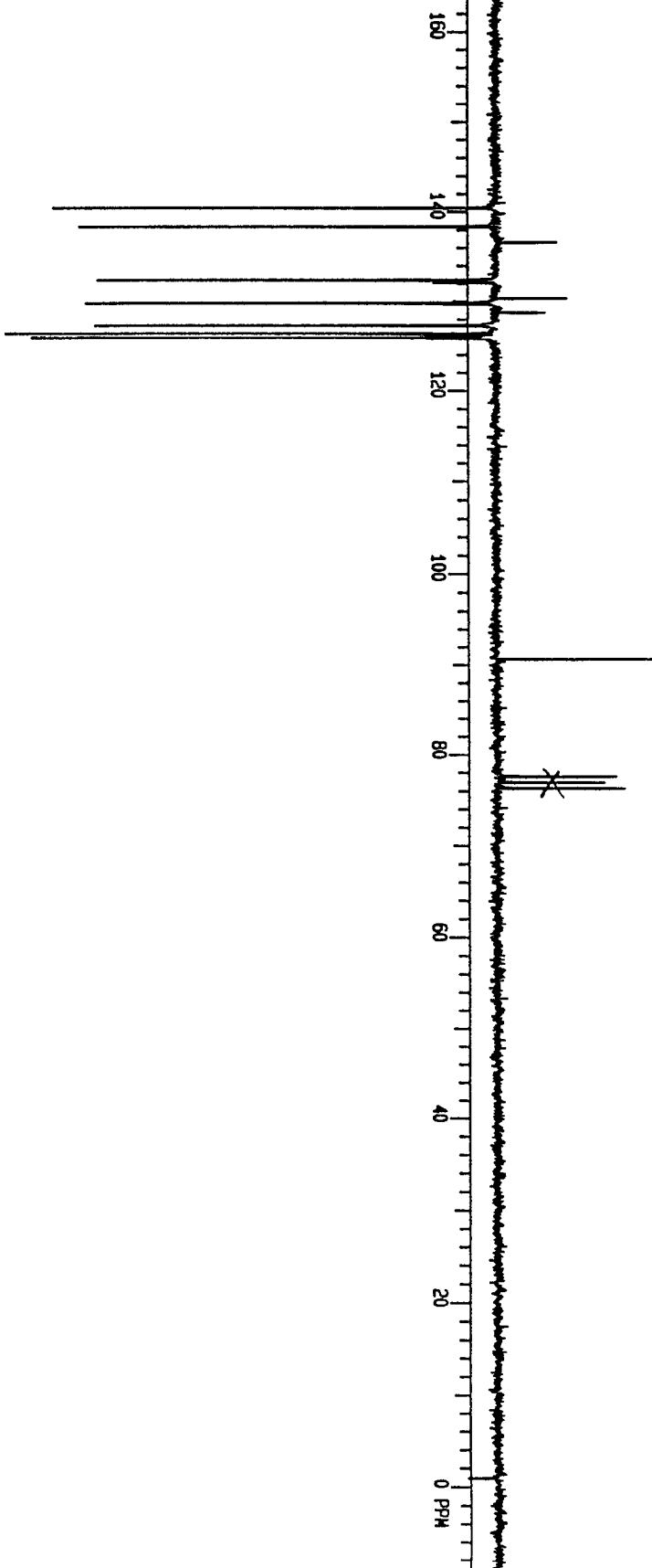


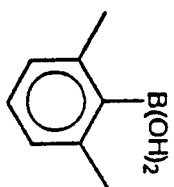


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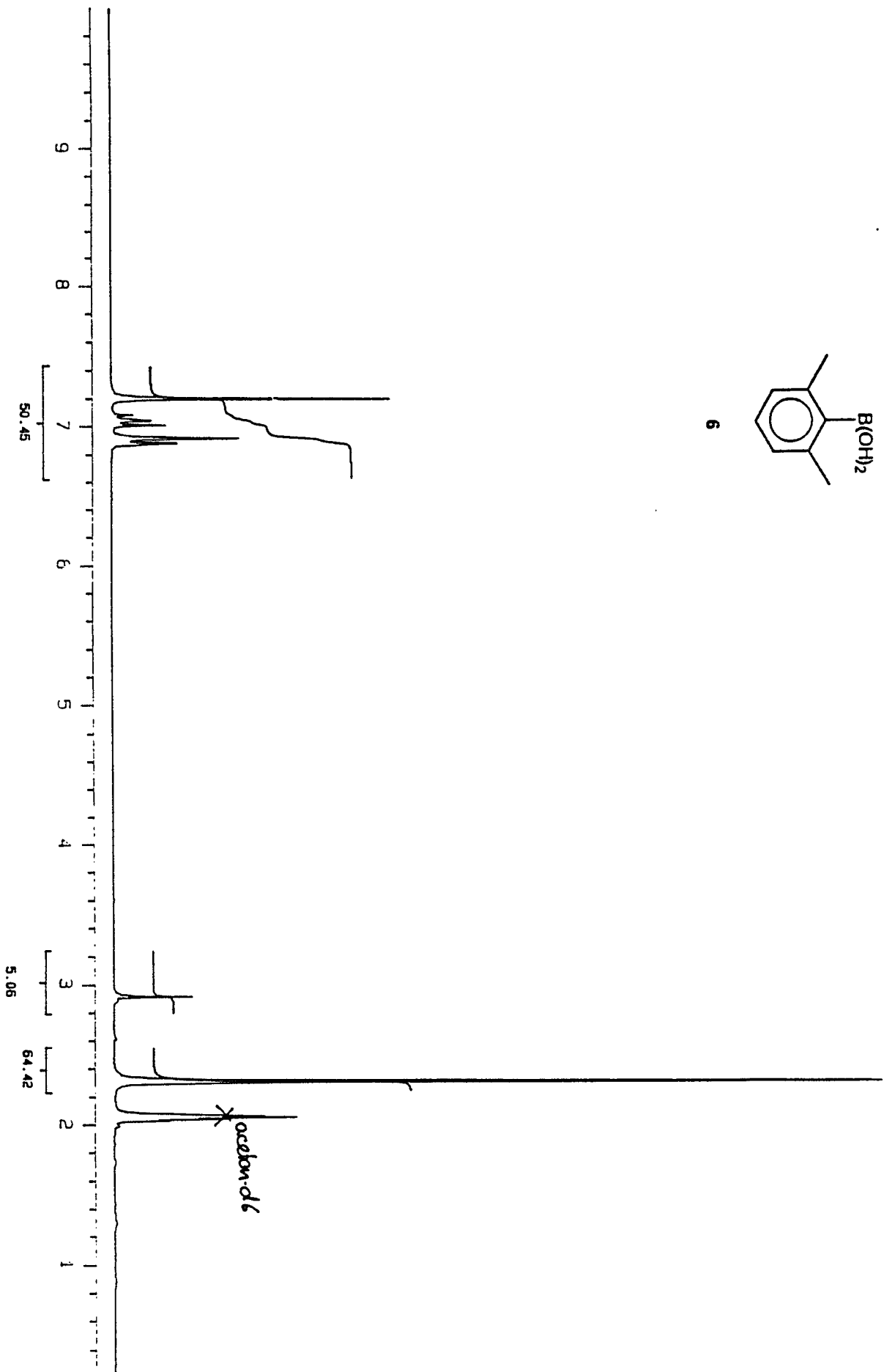


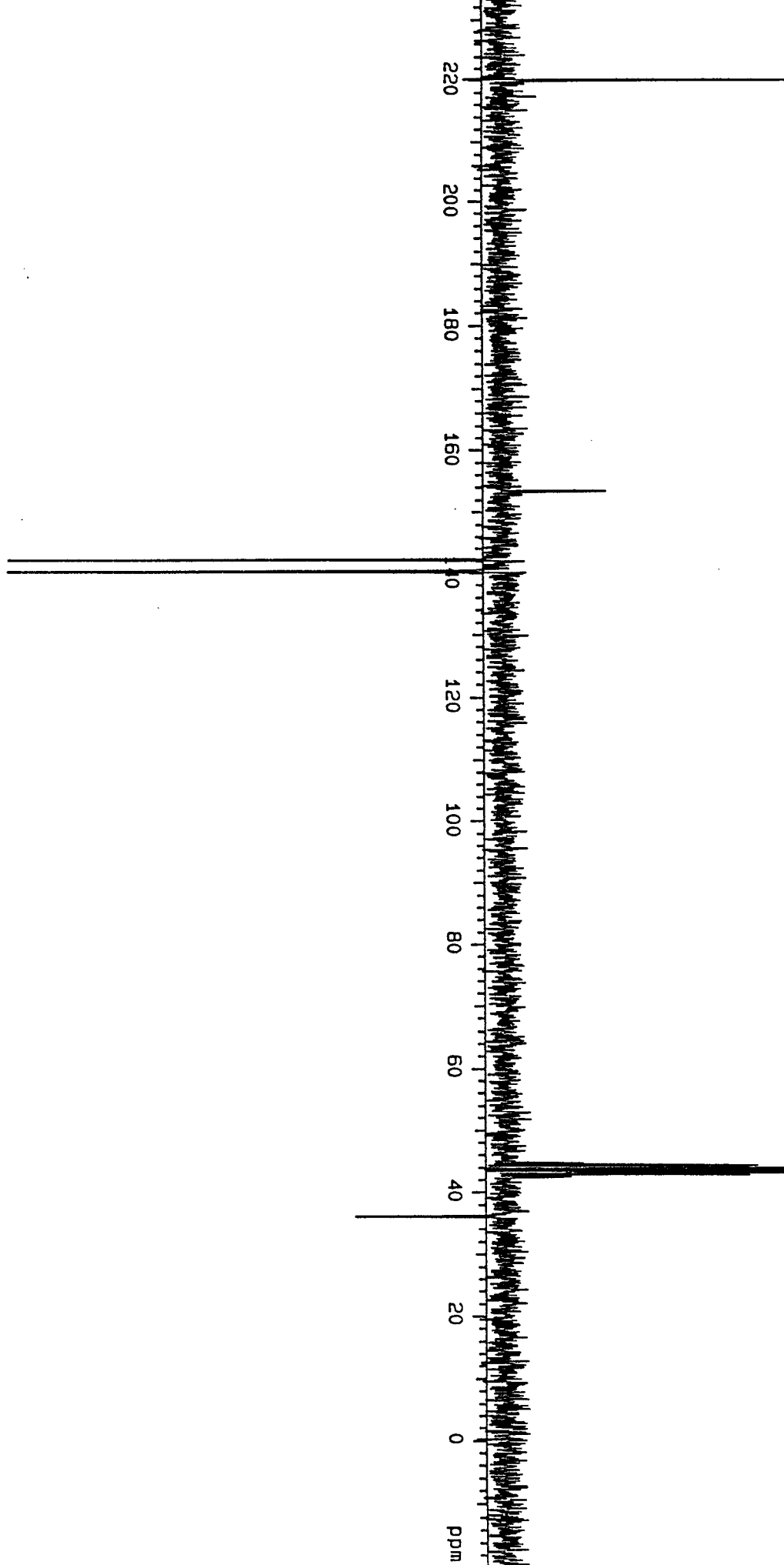
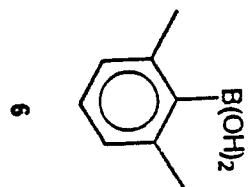
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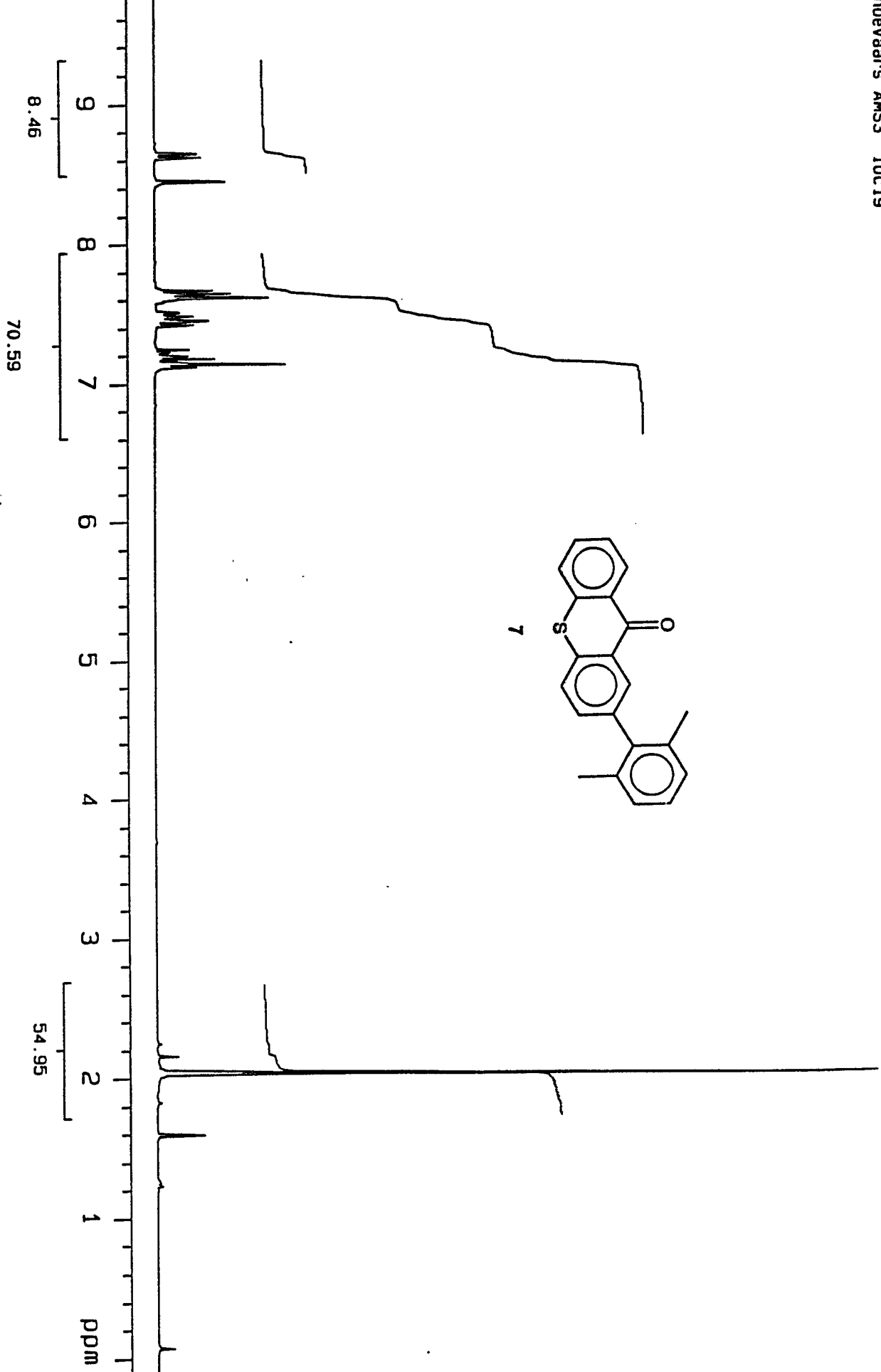
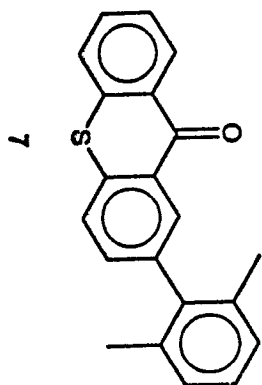




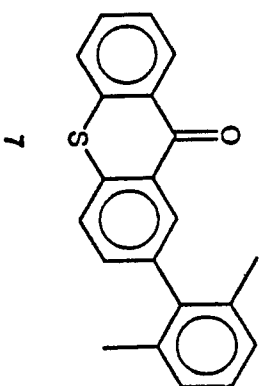
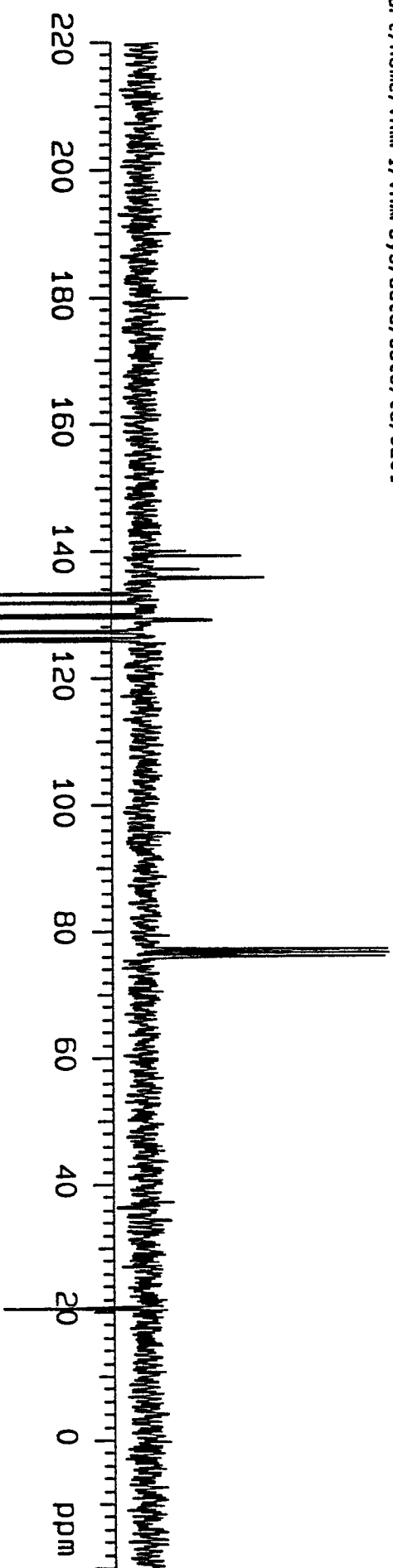
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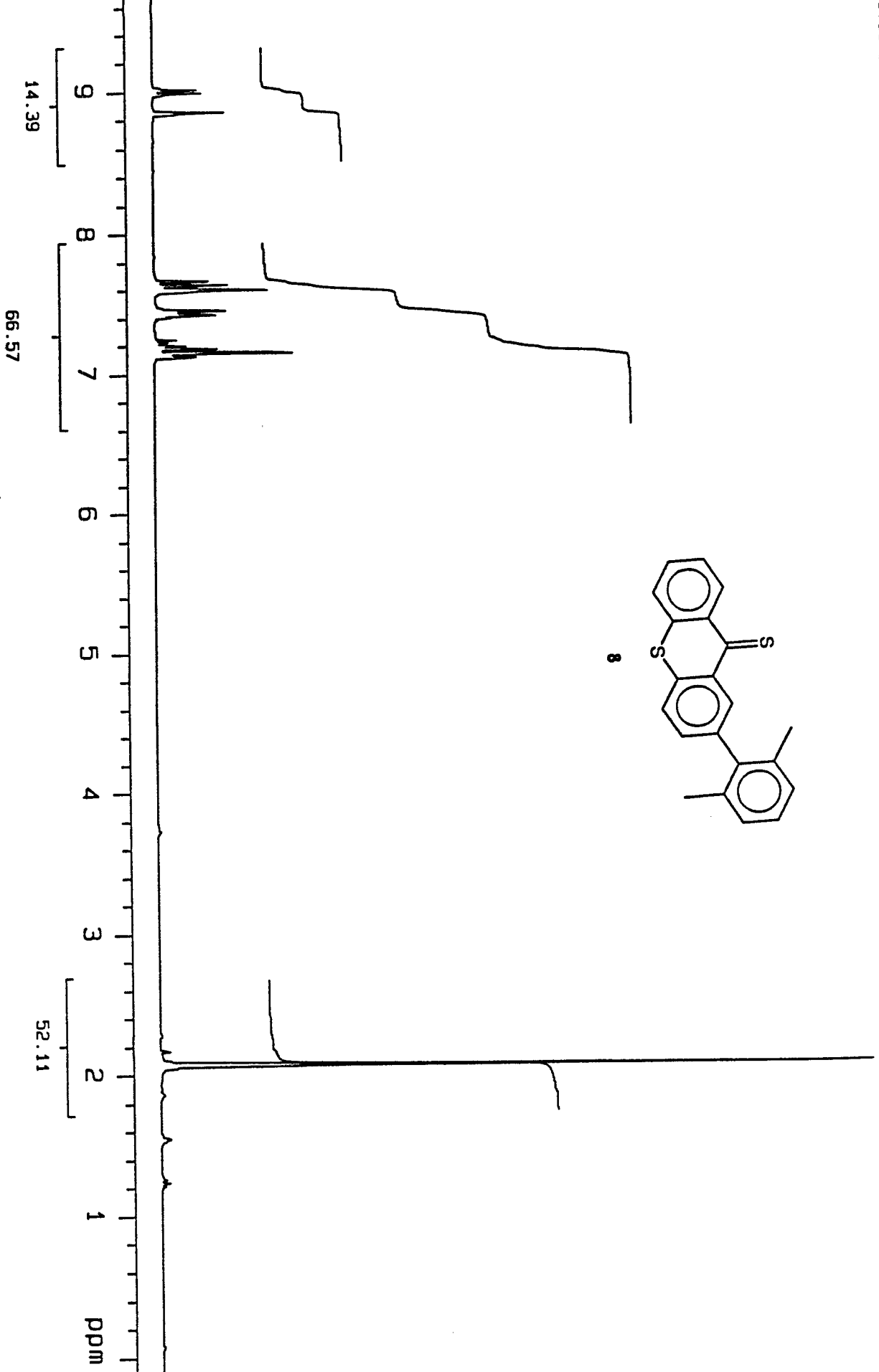
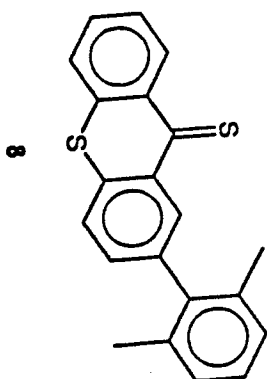






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TD: 65536

TE: 300.2

DELTA: 1.000

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NUC2: 1H

NUC3: 15N

NUC4: 19F

NUC5: 31P

NUC6: 12500.0 Hz

NUC7: 50.281249 MHz

NUC8: 199.968953 MHz

42 dB

16 modulated

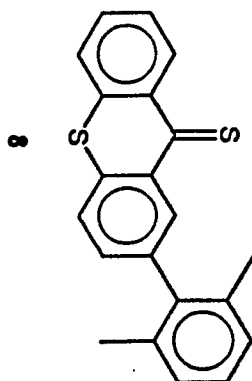
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32 minutes

65536

1.5 Hz

32 minutes



8

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